

4,5-Dibromo-1-methyl-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)-1H-pyrrole-2-carboxamide
113589-14-3 | DTXSID20556731

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.01

Global applicability domain: Inside

Local applicability domain index: 3.35e-01

Confidence level: 4.47e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4,5-Dibromo-1-methyl-3-
[(propan-2-yl)oxy]-N-(2H-tetrazol-
5-yl)-1H-pyrrole-2-carboxamide

Measured: 2.52

Predicted: 2.01

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4-Bromo-5-methoxy-3-[(propan-
2-yl)oxy]-N-(2H-tetrazol-5-
yl)thiophene-2-carboxamide

Measured: 1.35

Predicted: 1.66